2-Benzyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine 368441-96-7 | DTXSID50364048

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 8.42

Global applicability domain: Inside

Local applicability domain index: 9.39e-01

Confidence level: 8.60e-01

Nearest Neighbors from the Training Set

Image not found

1,2,3,4-Tetrachloronaphthalene

Measured: 8.30 Predicted: 8.41

Image not found

2,3-Dichlorodibenzo-4-dioxin

Measured: 8.50 Predicted: 8.49

Image not found

1,2,3,5-Tetrachloronaphthalene

Measured: 8.29 Predicted: 8.44